

## LA-UR-20-20056

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Title: SURF model calibration strategy

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Intended for: LANL seminar

Issued: 2020-01-06

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# SURF model calibration strategy



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January, 2020



Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

# Reactive burn model

## 1. EOS model

reactants, products

partially burned HE (mixture rule)

$P(V, e, \vec{\lambda})$  where  $\vec{\lambda}$  = reaction progress variable(s)

Tacitly assumes partly burned HE is homogeneous  
and in thermodynamic equilibrium

## 2. Reaction rates (empirical to account for heterogeneities)

Calibrate rate to detonation data

- Shock ignition regime

Pop plot data

Embedded gauge profiles

Complex loading conditions

- Propagation regime

Curvature effect

Failure diameter

# SURF model Rate

$\lambda$  is mass fraction of products

$s$  is reaction progress variable

$$\begin{aligned}\lambda &= g(s) \\ &= 1 - \exp(-s^2) \quad \text{cylindrical hot spots}\end{aligned}$$

$$s = [-\ln(1 - \lambda)]^{1/2}$$

$$ds/dt = \text{Rate}(P_s, P), \quad \underline{P_s = \text{lead shock pressure} \ \& \ P = \text{local pressure}}$$

$$= \begin{bmatrix} (P/P_s)^n & \text{for } P < P_s \\ (P/P_s)^{n_{hi}} & \text{for } P > P_s \end{bmatrix} \times \mathcal{R}(P_s)$$

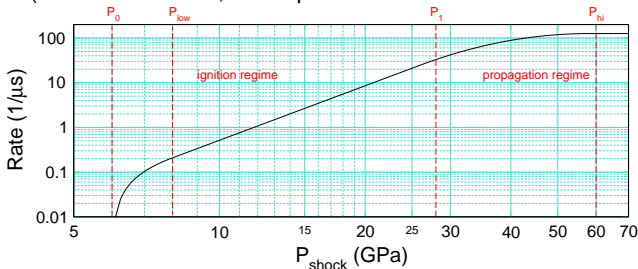
## Standard rate

$$\begin{aligned}(d/dt)\lambda &= (dg/ds) \times (ds/dt) \\ &= 2[-\ln(1 - \lambda)]^{1/2}(1 - \lambda) \times \text{Rate}(P_s, P)\end{aligned}$$

Cut-off for finite reaction zone:  $g(s_c) = 1$  at finite  $s_c$

# Rate $\mathcal{R}(P_s)$

Fitting form 4 (LA-UR-17-31015, SURFplus model calibration for PBX 9502)



## Pressure regions

$$P_s < P_0$$

rate=0, weak shock not effective at generating hot spots

$$P_0 < P_s < P_{\text{low}}$$

low pressure cutoff,  $\mathcal{R} = \tilde{C} (P_s - P_0)^{\tilde{n}}$

$$P_{\text{low}} < P_s < P_1$$

**ignition regime**,  $\mathcal{R} = C P_s^{f_n}$  to fit Pop plot data

$$P_1 < P_s < P_{\text{hi}}$$

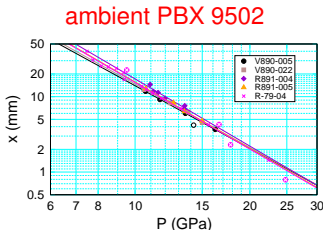
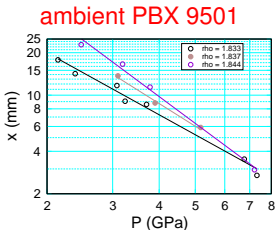
**propagation regime**, high pressure cutoff

$$P_{\text{hi}} < P_s$$

hot spots saturate (can add bulk thermal rate)

**Rate model has 8 parameters:**  $P_0, P_{\text{low}}, P_1, P_{\text{hi}}, C, f_n, n, n_{\text{hi}}$

# Shock ignition: Pop plot data



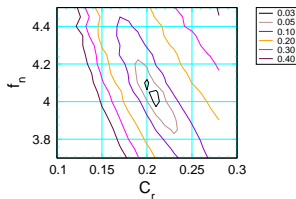
- **PBX 9501** variation with porosity
- **PBX 9502** variation with lot  
Large systematic variation with initial temperature (-55 and 75 C)
- **Scatter in data (6 % rms up to 30 % for outliers on log-log scale)**  
Experimental uncertainties and PBX heterogeneities  
Rate model can not accurately fit all data
- **Calibration data**  
Pop plot calibration should cover wide range in shock pressure

# Calibration to Pop plot data

Run distance from simulated lead shock pressure vs distance  
Pop plot dominated by 2 model parameters:  $C$  and  $f_n$

## Metric for calibration

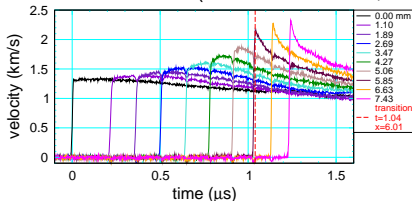
rms relative error of run distance relative to fit to Pop plot data



- Shallow trough in metric  
Correlated changes in  $C$  and  $f_n$  have small effect on metric
- Model Pop plot also affected by parameters  $n_{hi}$  and  $P_1$

# Embedded gauge data

PBX 9502 shot 2s86 (Gustavsen *et al.*, 2006)



- Transition-to-detonation should agree with fit to Pop plot data  
Subject to scatter in Pop plot data
- Shock rise time due to small mis-alignment of gauge package  
Gauge averages over about 1 cm transverse to propagation direction
- VN spike clipped due to response time of gauge (10 to 20 ns)
- Simulated shape of profiles depend on model function  $g(s)$  and parameter  $n_{hi}$

# Curvature effect experiments

## Unconfined rate stick

Diameter effect: axial detonation speed vs  $1/\text{radius}$

For curvature effect, also measure front shape

$D_n(\kappa)$  determined parametrically from derived  $\kappa$  and  $D_n$  along front

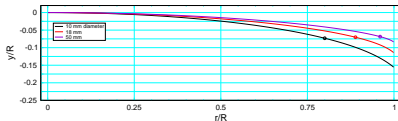
Issue: For large  $\kappa$ ,  $D_n$  depends on rate stick diameter

- **Boundary layer within 0.5 to 1 mm of HE/air interface**
  - At boundary lead shock is sonic and not supported by reaction along streamline
  - Large transverse pressure gradient along shock front
- **Assumptions of first order DSD theory break down**  
Outside boundary layer assumptions are valid
- **HE weakly confined for almost all applications**  
Due to gap/tolerance at HE/inert interface
- **Dependence on PBX lot  $\implies$  model uncertainty**

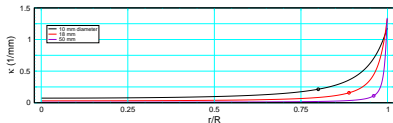
# Unconfined rate stick

PBX 9502 experiments by Larry Hill

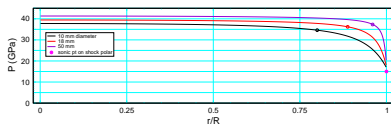
compare 3 diameters with normalized radius



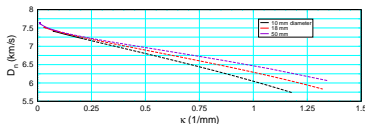
aspect ratio is 1 to 1  
circle 1 mm from boundary



$\kappa$  computed from front shape



$P$  based on reactants EOS and  
 $D_n$  computed from front shape



$D_n(\kappa)$  computed from front shape  
for  $\kappa > 0.25/\text{mm}$

$D_n$  depends on rate stick diameter  
corresponds to boundary layer

# Curvature effect calibration

For small to moderate  $\kappa$  (when assumptions of DSD theory hold)

- **ODEs for 1-D quasi-steady reaction zone profile**

Front curvature  $\kappa$  is parameter

Trajectory starts at lead shock

Singularity at sonic point ( $u + c = D$ ) unless  $\sigma\mathcal{R} = u\kappa$  (rate condition)

- **Shooting problem**

Vary  $D_n$  and evaluate trajectory

Until rate condition at sonic point is met

Solution exists only up to moderate  $\kappa$

- **Slope of  $D_n(\kappa)$  depends on reaction-zone width to sonic point**

Determined by rate in high pressure regime

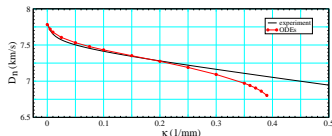
- **Extend ODEs to SURFplus fast/slow reactions**

$D_n(\kappa)$  curve has qualitatively different shape with carbon clustering

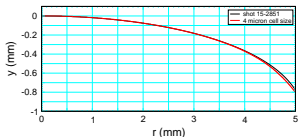
Alternatively, fast rate for  $\lambda < \lambda_{switch}$  and slow rate for  $\lambda > \lambda_{switch}$

# PBX 9502 curvature effect

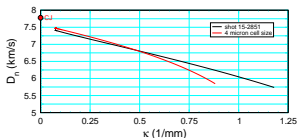
$D_n(\kappa)$  from ODEs



10 mm diameter rate stick (Larry Hill, shot 15-2851)  
xRage simulation with AMR to 0.004 mm

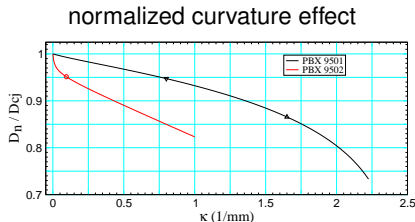


front shape (not to scale)

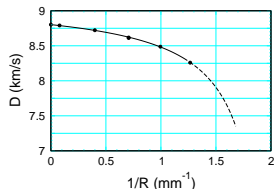


$D_n(\kappa)$  from front shape

# Curvature effect – fast/slow reaction



PBX 9501 diameter effect



- PBX 9501 – fast reaction only**

Failure diameter less than 1.6 mm

Black triangles: bounds for diameter effect limiting detonation speed

DSD needs  $D_n(\kappa)$  to extend to smaller  $D_n$  than limiting  $D_n$

- PBX 9502 – fast/slow reaction**

Failure diameter approximately 9 mm

As  $\kappa$  increases: sonic point goes from end of slow to end of fast reaction

large change in reaction-zone width to sonic point

Red circle: detonation speed for 1 inch cylinder test

# Failure diameter and front shape

## 2-D simulations of unconfined rate stick

Experiments used to determine  $D_n(\kappa)$  and front shape

- **Computationally expensive compared to 1-D shock initiation**

Need to resolve reaction zone

Cylinder length at least 4 diameters

Iterate to fit failure diameter and limiting detonation speed

- **Parameter  $n$  and SURFplus rate**

$n$  affects reaction-zone width and failure (but not Pop plot)

Lower rate for pressure decreasing gradient behind front

Important for non-planar shock initiation (fragment impact)

SURFplus slow rate important for curvature effect and failure

- **Fit shape of detonation front**

More robust to fit front shape than  $D_n(\kappa)$  for large  $\kappa$

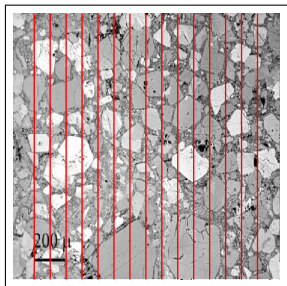
since  $\kappa$  depends on first and second derivative of front shape

Due to boundary layer, front shape more fundamental than  $D_n(\kappa)$

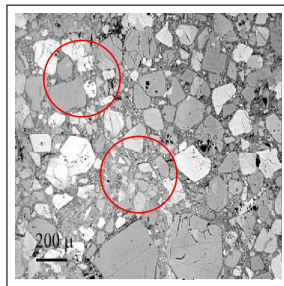
# ZND reaction-zone profile

Experiments to measure 1-D reaction-zone profile have been tried  
Large shot-to-shot variation in VN spike and reaction-zone width

Polarized light micrograph of PBX 9501 [Skidmore *et al.*, 1998]



reactive HE  
burn models  
treat PBX as  
homogeneous



Red lines 100 microns apart  
Estimated reaction-zone width  
25 to 75 microns < av grain size  
Expect reaction-zone profile to vary  
with local grain/binder variations

Red circles PDV probe spot size  
500 micron diameter  
Velocity varies over spot size  
Number of grains small & variable  
Profile varies due to poor statistics